

Interim Standard Chemical Identification Data Elements

The standard specifies the key data elements necessary to constitute a viable chemical substance record. It is based on the Chemical Abstracts Service (CAS) registry numbering standard but also includes additional identification elements. This standard requires that a complete record be centrally created and maintained.

Mandatory Data Elements for Interim Chemical Identification Standard			
Data Element	Definition	Notes	EDR DE ID
Chemical Abstracts Service Registry Number	The unique number assigned by Chemical Abstracts Service (CAS) to a chemical substance.		6165:1
Chemical Substance Systematic Name	The name assigned to a chemical substance that describes it in terms of its molecular composition.	The preferred name is the index name formulated according to the Chemical Abstracts Service 9th Collective Index Nomenclature Standard.	5799:1
EPA Chemical Registry Name	The name that the Environmental Protection Agency has selected as its preferred name for a chemical substance.		5801:1
EPA Chemical Identification Number	The unique identifier assigned to a chemical substance for Environmental Protection Agency use.	This is the unique record number for the Chemical Substance.	20040:1

Optional Data Elements for Interim Chemical Identification Standard

Data Element	Definition	Notes	EDR DE ID
Chemical Synonym Context Name	The name that identifies the circumstances for which a chemical substance name is used.		20042:1
EPA Chemical Registry Name Source	The source of the Environmental Protection Agency chemical registry name.		20048:1
EPA Chemical Registry Name Context	The type of source for the Environmental Protection Agency chemical registry name.		20052:1
Chemical Substance Definition Text	The text that provides clarification to the identity of a chemical substance.		20055:1
Chemical Substance Comment Text	The text that provides additional information about a chemical substance.		20056:1
Chemical Substance Synonym	A name that is used as the alternative for representing a chemical substance.	A synonym can be a name or identification number used currently or historically to identify the chemical substance.	5806:1
Molecular Formula Code	The code that represents the number of atoms of each element in a molecule of a chemical substance.		5812:1
Chemical Substance Formula Weight Quantity	The sum of the atomic weights of constituent atoms in a molecule of a chemical substance.		5814:1
Chemical Substance Type Name	A descriptive name for types of chemical substances.		5818:1

Chemical Substances Linear Structure Code	The code that represents the connectivity of atoms in a molecule of a chemical substance as a linear formula, such as SMILES.		26069:1
Chemical Structure Graphical Diagram	A graphical representation of a molecule of a chemical substance as a two or three dimensional diagram.		26070:1
Chemical Substance Classification Name	The name of a schema that classifies chemical substances according to structural similarities.		26072:1
Chemical Synonym Status Name	The name that documents the correctness of a synonym for a specific chemical substance.		26071:1
Chemical Synonym Source Name	The name of the source of an alternate name for a chemical substance.		26073:1